Dimefox
115-26-4 | DTXSID8041870

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.54

Global applicability domain: Inside

Local applicability domain index: 4.44e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

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Trimethyl phosphate
Measured: 1.41
Predicted: 1.50

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Benzenesulfonamide
Measured: 4.79
Predicted: 2.10

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1,1'-Oxybis-2-propanol
Measured: 4.57
Predicted: 3.83

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o-Toluenesulfonamide
Measured: 2.57
Predicted: 2.00

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Triethyl phosphate
Measured: 1.29
Predicted: 1.38